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14. ABSTRACT

These Lecture Series was dedicated to numerical description of nanoparticles in a fluid. Different possible frameworks were reviewed including Lagrangian, Eulerian, continuous or non-continuous approach
A complete description of the Method of Moments with Interpolative Closure together with the Dynamic Monte Carlo technique combine with atomistic model allowed describing the nanoparticle formation from its nucleation to its aggregation.

Review of alternative approach such as the multi-fluid formulation derived from the Kinetic theory is done. A complete description of electrostatic effect including the transport, deposition and removal of charged nanoparticles plus the static and the dynamic electrorheology presentation are done. Many other advance processes including the sintering phenomenon treated with the stochastic particle method and applied to the soot formation are proposed. The transport properties of plasma flows are reviewed in order to better understand the nanoparticle synthesis from a plasma reactor. Among other this synthesis must use an efficient quench in order to condense the chemical species in a cloud of nanoparticle nucleus.

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RTO EDUCATIONAL NOTES **EN-AVT-169**

Modeling and Computation of Nanoparticles in Fluid Flows

(Modélisation et calcul des nanoparticules dans la circulation des fluides)

Papers presented at the AVT-169 RTO AVT/VKI Lecture Series held at the von Karman Institute, Rhode St. Genèse, Belgium, 9-12 February 2009.

Published February 2009

The Research and Technology Organisation (RTO) of NATO

RTO is the single focus in NATO for Defence Research and Technology activities. Its mission is to conduct and promote co-operative research and information exchange. The objective is to support the development and effective use of national defence research and technology and to meet the military needs of the Alliance, to maintain a technological lead, and to provide advice to NATO and national decision makers. The RTO performs its mission with the support of an extensive network of national experts. It also ensures effective co-ordination with other NATO bodies involved in R&T activities.

RTO reports both to the Military Committee of NATO and to the Conference of National Armament Directors. It comprises a Research and Technology Board (RTB) as the highest level of national representation and the Research and Technology Agency (RTA), a dedicated staff with its headquarters in Neuilly, near Paris, France. In order to facilitate contacts with the military users and other NATO activities, a small part of the RTA staff is located in NATO Headquarters in Brussels. The Brussels staff also co-ordinates RTO's co-operation with nations in Middle and Eastern Europe, to which RTO attaches particular importance especially as working together in the field of research is one of the more promising areas of co-operation.

The total spectrum of R&T activities is covered by the following 7 bodies:

- AVT Applied Vehicle Technology Panel
- HFM Human Factors and Medicine Panel
- IST Information Systems Technology Panel
- NMSG NATO Modelling and Simulation Group
- SAS System Analysis and Studies Panel
- SCI Systems Concepts and Integration Panel
- SET Sensors and Electronics Technology Panel

These bodies are made up of national representatives as well as generally recognised 'world class' scientists. They also provide a communication link to military users and other NATO bodies. RTO's scientific and technological work is carried out by Technical Teams, created for specific activities and with a specific duration. Such Technical Teams can organise workshops, symposia, field trials, lecture series and training courses. An important function of these Technical Teams is to ensure the continuity of the expert networks.

RTO builds upon earlier co-operation in defence research and technology as set-up under the Advisory Group for Aerospace Research and Development (AGARD) and the Defence Research Group (DRG). AGARD and the DRG share common roots in that they were both established at the initiative of Dr Theodore von Kármán, a leading aerospace scientist, who early on recognised the importance of scientific support for the Allied Armed Forces. RTO is capitalising on these common roots in order to provide the Alliance and the NATO nations with a strong scientific and technological basis that will guarantee a solid base for the future.

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Modeling and Computation of Nanoparticles in Fluid Flows

(RTO-EN-AVT-169)

Executive Summary

These Lecture Series proceedings are especially dedicated to the numerous topics arising when researchers have to predict numerically the behaviour of nanoparticles in a fluid. Beside an isolated nano object, the keyword of nanoparticle has to be understood more generally as including also agglomerate of nanoparticles, of nano-tubes and/or related complex structures.

As a matter of fact, numerous questions arise when the formation and the path of such objects have to be numerically predicted. Already concerning the methodology, the researchers have to select a Lagrangian or an Eulerian framework for the models development. The applicability of some of these models may be questionable when the diameter of the nanoparticles is comparable to the local molecular mean free path. In other words, it may be crucial to choose between a continuous and a non-continuous approach.

These two important issues are presented in the proceedings together with many others such as a detailed introduction to the Method of Moments with Interpolative Closure (MOMIC). It is shown how this method may be combined with the Dynamic Monte Carlo (DMC) technique allowing the study of nanoparticles aggregation. MOMIC, DMC and atomistic modeling allow also studying the particle formation from its nucleation including the particle surface growth.

These Lecture Series proceedings also include a complete description of the multi-fluid formulation extracted from the Kinetic theory with details on different models such as the one describing coalescence. The transport, deposition and removal of charged nanoparticles are also investigated together with a full detailed presentation of the static and the dynamic electrorheology approach. The sintering process of nanoparticles is presented in the frame of stochastic particle method and applied to the soot formation. The transport properties of plasma flows are reviewed in order to better understand the nanoparticle synthesis from a plasma reactor. This approach uses an efficient quench in order to condense the chemical species in a cloud of nanoparticle nucleus.

All these advanced models, methods and techniques are presented and detailed by a panel of distinguished authors worldly recognized for their contributions in numerical models for nanoparticles in fluids.

Modélisation et calcul des nanoparticules dans la circulation des fluides

(RTO-EN-AVT-169)

Synthèse

Ces minutes du cycle de conférences sont spécialement consacrés aux nombreux sujets de discussion qui apparaissent lorsque les chercheurs doivent prédire numériquement le comportement des nanoparticules dans un liquide. Au-delà du nano-objet isolé, le mot clé de nanoparticule doit aussi être compris plus généralement comme incluant des agglomérats de nanoparticules, de nanotubes et/ou les structures complexes associées.

En fait, de nombreuses questions surgissent lorsqu'il s'agit de faire une prédiction numérique sur la formation et le parcours de tels objets. En ce qui concerne déjà la méthodologie, les chercheurs doivent choisir entre une structure de Lagrange et une structure d'Euler pour le développement des modèles. L'applicabilité de certains de ces modèles peut être discutable quand le diamètre des nanoparticules est comparable à la trajectoire libre moléculaire locale moyenne. En d'autres termes, il peut être crucial de choisir entre une approche continue ou discontinue.

Ces deux importantes questions sont présentées dans les comptes-rendus entre d'autres nombreuses questions comme l'introduction détaillée de la Méthode des Moments avec Fermeture par Interpolation (MOMIC). On démontre comment cette méthode peut être combinée avec la technique Dynamic Monte Carlo permettant l'étude de l'agrégation des nanoparticules. Le MOMIC, le DMC et la modélisation atomistique permettent aussi d'étudier la formation des particules à partir de leur noyau en incluant le développement de la surface de la particule.

Ces comptes-rendus du cycle de conférences contiennent aussi une description complète de la formulation multi fluides extraite de la théorie cinétique avec des détails sur différents modèles comme celui qui décrit la coalescence. Le transport, le dépôt et l'élimination des nanoparticules chargées sont aussi étudiés avec une présentation détaillée complète de l'approche électro-rhéologique statique et dynamique. Le processus de frittage des nanoparticules est présenté dans le cadre de la méthode stochastique des particules et appliqué à l'encrassement. Les propriétés du transport par flux de plasma sont étudiées pour avoir une meilleure compréhension de la synthèse des nanoparticules à partir d'un réacteur à plasma. Cette approche utilise un refroidissement brusque de façon à condenser les substances chimiques dans un nuage de noyaux de nanoparticules.

Tous ces modèles, ces méthodes et ces techniques évolués sont présentés et détaillés par un ensemble d'auteurs réputés reconnus mondialement pour leur contribution dans les modèles numériques sur les nanoparticules dans les fluides.

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